

**PROGRAM**  
**“ADVANCES IN TRANSITION METAL CATALYZED REACTIONS”**  
**Monday, October 22, 2012**

8:30 **WILHELMINA E. ROBERTSON**, Chairman of the Board of Directors  
8:35 **RICHARD R. SCHROCK**, Massachusetts Inst. of Technology, Program Chairman

**SESSION I -**

---

8:40 **JOHN A. GLADYSZ**, Texas A&M University, Discussion Leader

8:50 **DANIEL G. NOCERA**, Massachusetts Institute of Technology,  
*“The Artificial Leaf”*  
Discussion

9:40 **ROY A. PERIANA**, The Scripps Research Institute,  
*“The Design and Study of Molecular Catalysts for Strong Bond Activation and Conversion”*  
Discussion

10:30 Break

10:45 **GEOFFREY W. COATES**, Cornell University,  
*“Bimetallic Catalysis: Design, Discovery, and Applications in Organic and Materials Chemistry”*  
Discussion

11:35 LUNCH

**SESSION II**

---

1:00 **RICHARD F. JORDAN**, University of Chicago, Discussion Leader

1:10 **RICHARD R. SCHROCK**, Massachusetts Institute of Technology,  
*“Molybdenum and Tungsten Catalysts for Selective Olefin Metathesis Reactions”*  
Discussion

2:00 **PAUL J. CHIRIK**, Princeton University,  
*“Modern Alchemy: The Chemistry of Base Metal Catalysis”*  
Discussion

2:50 Break

3:05 **CHRISTOPHE COPÉRET**, ETH Zürich,  
*“Controlled Functionalization of Surfaces: Supported Single-Site Catalysts and Beyond”*  
Discussion

4:00 Adjourn

**Tuesday, October 23, 2012**

**SESSION III**

---

- 8:00 **MICHAEL J. KRISCHE**, The University of Texas at Austin, Discussion Leader
- 8:10 **AMIR H. HOVEYDA**, Boston College,  
*“New Concepts, Catalysts and Methods for Stereoselective Synthesis of Alkenes. Mechanistic Insights and Applications to Complex Molecule Synthesis”*  
Discussion
- 9:00 **F. DEAN TOSTE**, University of California, Berkeley,  
*“Enantioselective Catalysis with Gold Complexes”*  
Discussion
- 9:50 Break
- 10:05 **VY M. DONG**, University of Toronto,  
*“A Few of My Favorite Rings: Catalysis Inspired by Lactones and Lactams”*  
Discussion

**2012 Welch Awardee Lecture**

---

- 10:55 **DAVID A. EVANS**, Harvard University,  
*“Polycyclic Structures from Macrocyclic Intermediates”*
- 11:35 LUNCH

**SESSION IV**

---

- 1:00 **JOHN E. BERCAW**, California Institute of Technology, Discussion Leader
- 1:10 **MARCETTA Y. DARENSBOURG**, Texas A&M University,  
*“Molecular Constructs as [FeFe]-H<sub>2</sub>ase Enzyme Active Site Biomimetics for Proton Reduction”*  
Discussion
- 2:00 Break
- 2:15 **JIN-QUAN YU**, The Scripps Research Institute,  
*“Accelerated C-H Activation Reactions: A Shortcut to Drug Molecules from Chemical Feedstock”*  
Discussion
- 3:05 **MAURICE BROOKHART**, University of North Carolina at Chapel Hill,  
*“Applications of Iridium Pincer Complexes in Catalysis: Hydrocarbon Conversions”*  
Discussion
- 4:00 Adjourn



## JOHN A. GLADYSZ

Texas A&M University

Monday, October 22, 2012; 8:40 AM

Professor Gladysz is a fellow of the Alfred P. Sloan Foundation (1980-1984) and a Camille and Henry Dreyfus Teacher-Scholar Grant recipient (1980-1985). He has been honored nationally with two prizes from the American Chemical Society: the Arthur C. Cope Scholar Award (1988) and the Award in Organometallic Chemistry (1994). In 1995, he received an Alexander von Humboldt Foundation Research Award for Senior Scientists. From 1984 until 2010, he was the Associate Editor of *Chemical Reviews*, the journal

with the highest impact factor in chemistry. Dr. Gladysz is the Editor in Chief of *Organometallics* since 2010.

Professor Gladysz's research centers around organometallic chemistry, and from this core branches into nanotechnology, stereochemistry, organic synthesis, enantioselective reactions, catalysis, mechanism, and materials chemistry. This work has been described in over 400 widely-cited publications.



## DANIEL G. NOCERA

Massachusetts Institute of Technology  
Monday, October 22, 2012; 8:50 AM

Daniel G. Nocera is the Henry Dreyfus Professor of Energy at the Massachusetts Institute of Technology, Director of the Solar Revolutions Project and Director of the Eni Solar Frontiers Center at MIT. His group pioneered studies of the basic mechanisms of energy conversion in biology and chemistry. He has recently accomplished a solar fuels process that captures many of the elements of photosynthesis and he has now translated this science to produce an artificial leaf, which was named by *Time Magazine* as Innovation of the Year for 2011. This discovery sets the stage for a storage mechanism for the large scale, distributed, deployment of solar energy. He has been awarded the Eni Prize, IAPS Award, Burghausen Prize, Elizabeth Wood Award and the United Nation's Science and Technology Award and from the American Chemical Society the Awards in Inorganic Chemistry, Harrison Howe and Remsen Awards, for his contributions to the development of renewable energy. He is a member of the American Academy of Arts and Sciences and the U.S. National Academy of Sciences. He was named as 100 Most Influential People in the World by *Time Magazine* and was 11th on the *New Statesman's* list on the same topic. Nocera is a frequent guest on TV and radio, he is regularly featured in print and he was in the feature length film *Cool It*, which premiered in the U.S. in November 2010. His 2006 PBS show was nominated for an Emmy Award, and the show was used as a pilot to launch the PBS NOVA show, *ScienceNow*. In 2008, he founded Sun Catalytix, a company committed to bringing personalized energy to the non-legacy world.

### **Abstract: The Artificial Leaf**

It has been said for an ideal solar fuels process that the system requirements are:

- ❖ Earth-abundant materials
- ❖ No wires
- ❖ Direct solar-to fuels process.

Two earth abundant catalysts have been discovered that promote the oxygen evolving reaction (OER) and hydrogen evolving reaction (HER). The ability to operate these catalysts under benign conditions (in water at pH 7 and under 1 atm) has enabled the construction of the artificial leaf, which consists of a silicon wafer, coated with the respective OER and HER catalysts. By immersing the artificial leaf in water and holding it up to sunlight causes efficient water splitting; and all of this is done with no wires. The system surpasses the prescription from the community because it also does not rely on a membrane. By constructing a simple, stand-alone device composed of earth-abundant materials, the artificial leaf provides a means for an inexpensive and distributed direct solar-to-fuels conversion process with low-cost systems engineering and manufacturing requirements. The science behind the catalysts and the artificial leaf will be presented.



## ROY A. PERIANA

The Scripps Research Institute  
Monday, October 22, 2012; 9:40 AM

Prof. Roy A. Periana completed his Ph.D. work under the supervision of Prof. Robert G. Bergman at the Univ. of California Berkeley (1985). As an industrial chemist, he has worked at Dow Chemical Co. (1979-1981), Monsanto Company (1985-1988), as a group leader at Catalytica Inc., (1988) and was a co-founder and vice president of research at Catalytica Advanced Technologies (1994). He then joined the Chemistry Dept. at the Univ. of Southern California (USC) (2000). During his time at USC, he was a member of the Loker Hydrocarbon Institute and Director for the USC-Caltech-Chevron consortium on catalysis. Since 2001, Prof. Periana has been a visiting associate in the Chemistry Dept. at the California Institute of Technology. He was a co-founder and served on the board of directors for Qateomix (2005). In 2007, he was appointed Professor and Director of the Scripps Energy and Materials Center (SEMC) at The Scripps Research Institute (TSRI). During his career he authored many articles and chapters that have been published in notable journals such as *Science* and covered in *Chemical and Engineering News*, *The Wall Street Journal*, and *The New York Times*. He has been an invited speaker at numerous national and international conferences. His current interest is on the design of catalysts for the low temperature, selective, conversion of small molecules with emphasis on CH<sub>4</sub>, CO<sub>2</sub> and N<sub>2</sub>.

### **Abstract: The Design and Study of Molecular Catalysts for Strong Bond Activation and Conversion**

New chemistry for strong bond could help to address the energy security and sustainability challenges. Catalysts in strongly acidic media that operate by electrophilic C-H activation/LM-R oxy-functionalization mechanisms facilitate the direct, selective conversion of strong alkane R-H bonds to R-OH bonds. In addition to increasing reaction rate, a key role of the acid media is to maximize selectivity by generating R-OH<sub>2</sub><sup>+</sup> that is "protected" from electrophilic reactions. We believe that this type of "protection" strategy may be required for direct, selective methane conversion. To address the practical limitations of these initial systems we are exploring the design of new catalysts that operate by CH activation/LM-R oxy-functionalizations that do not require strongly acidic media. A simplified conceptual basis for the low reactivity of strong bonds is the large HOMO-LUMO gaps. This model would suggest that there could be three electronically distinct CH activation reactions with electrophilic, ambiphilic and nucleophilic character. The key characteristic differences of these reactions could be the generation of positive, neutral and negative charges, respectively, on the carbon in the transition states for C-H cleavage. We are particularly interested in designing catalysts that operate by nucleophilic CH activation mechanisms to generate LM-R<sup>δ-</sup> type intermediates. These systems could plausibly operate in strongly basic media where ROH could be "protected" by deprotonation to RO<sup>-</sup>. While it may seem counter intuitive that CH activation could be carried out in strongly coordinating, basic media, we have now developed several new systems with non-innocent, protic ligands and electron-rich, d<sup>6</sup> metals (Ru<sup>II</sup>, Rh<sup>III</sup>, Ir<sup>III</sup>, etc.) that show H/D exchange with CH<sub>4</sub> and C<sub>6</sub>H<sub>6</sub> in aqueous KOH. We postulate, and calculations support, that reversible deprotonation of the non-innocent protic ligands generates highly nucleophilic, labile complexes that can cleave CH bonds to generate LM-R<sup>δ-</sup> intermediates. To address the lack of known oxy-functionalization reactions of LM-R<sup>δ-</sup> intermediates we have now shown that model Re<sup>VII</sup>-R and Re<sup>I</sup>-R complexes can be readily converted to ROH by reactions with O-atom donors in basic media. The current focus is on the integration of the nucleophilic CH activation and LM-R<sup>δ-</sup> functionalization steps into complete catalytic systems. We are exploring various strategies to address a key challenge involving catalyst deactivation by over oxidation of the electron-rich metal center. To explore the scope of reactions of these nucleophilic catalysts generated in basic media we have begun to investigate the activation and functionalization reactions with other strong bonds such as N=N and C-F.



## GEOFFREY W. COATES

Cornell University

Monday, October 22, 2012; 10:45 AM

Geoffrey W. Coates was born in 1966 in Evansville Indiana. He received a B.A. degree in Chemistry from Wabash College in 1989 and a Ph.D. in Organic Chemistry from Stanford University in 1994. His thesis work, under the direction of Robert M. Waymouth, investigated the stereoselectivity of metallocene-based Ziegler-Natta catalysts. Following his doctoral studies, he was an NSF Postdoctoral Fellow with Robert H. Grubbs at the California Institute of Technology. During the summer of 1997 he joined the faculty of

Cornell University as an Assistant Professor of Chemistry. He was promoted to Associate Professor in 2001, and to Professor in 2002. He was appointed to the first Tisch University Professorship in 2008.

The research focus of the Coates Group is the development of new catalysts for the synthesis of macromolecules as well as small molecules. Professor Coates' research concentrates on developing new methods for reacting commodity feedstocks in unprecedented ways. His current research centers on the development of homogeneous catalysts for olefin polymerization, heterocycle carbonylation, epoxide homo- and copolymerization, and the utilization of carbon dioxide in polymer synthesis.

Professor Coates is an Alfred P. Sloan Research Fellow, and has received awards from the ACS (A. C. Cope Scholar Award, Affordable Green Chemistry Award, A. K. Doolittle Award, Carl S. Marvel - Creative Polymer Chemistry Award, and Akron Section Award), NSF (CAREER), MIT Technology Review Magazine (TR 100 Award), Research Corporation (Innovation Award), Arnold and Mabel Beckman Foundation (Young Investigator Award), David and Lucile Packard Foundation (Fellowship in Science and Engineering), and Dreyfus Foundation (Camille and Henry Dreyfus New Faculty and Camille Dreyfus Teacher-Scholar Awards). In 2006, he received the Stephen and Margery Russell Distinguished Teaching Award at Cornell University and became a member of the American Association for the Advancement of Science. In 2011 he was identified by Thomson Reuters as one of the world's top 100 chemists on the basis of the impact of his scientific research, and was inducted into the American Academy of Arts & Sciences. He is the scientific cofounder and CSO of Novomer Inc., and is a member of the Scientific Advisory Board of KensaGroup. He is a member of the editorial advisory boards of the *Journal of Polymer Science*, *Chemical Reviews*, and *ChemCatChem*. He is a member of the Editorial Board of *Dalton Transactions*, and is an Associate Editor of *Macromolecules*.

### **Abstract: Bimetallic Catalysis: Design, Discovery, and Applications in Organic and Materials Chemistry**

At the current time, society depends on polymeric materials more than at any other time in history. Although synthetic polymers are indispensable in a diverse array of applications, ranging from commodity packaging and structural materials to technologically complex biomedical and electronic devices, their synthesis and post-use fate pose important environmental challenges. The focus of our research is the development of routes to polymers with reduced environmental impact. We aim to transition from fossil fuels to renewable resources, and are developing synthetic methods that limit energy and raw-material consumption. In addition, we are designing materials that will eventually degrade into non-toxic materials, and have properties comparable to current commodity plastics.

To achieve these goals, we have developed a range of metal based catalysts, many of which benefit by the presence of two metal centers. These bimetallic catalysts act in concert to create new mechanistic pathways for organic and materials synthesis. In this lecture, the development of catalytic routes to polyolefins, polyesters, polycarbonates, and polyethers will be presented.



## RICHARD F. JORDAN

University of Chicago

Monday, October 22, 2012; 1:00 PM

Richard Jordan is Professor and Chairman of the Department of Chemistry at the University of Chicago. He received his training in chemistry at Rutgers University (B.A., 1975) and Princeton University (Ph.D., 1981), and was a postdoctoral fellow at the University of Wisconsin (1981-83). He was a research chemist at Arco Chemical (1975-76) and served on the faculties of Washington State University (1983-87) and the University of Iowa (1988-99) prior to moving to Chicago in 1999.

Jordan's research focuses on organometallic chemistry, catalysis and polymers. He was among the first to recognize that the active species in metallocene-catalyzed olefin polymerizations are cationic d-zero metal alkyls. He prepared stable cationic d-zero zirconocene alkyl complexes and demonstrated that these species polymerize olefins. His studies of the synthesis and reactivity of d-zero metal alkyl and olefin complexes provided a deep understanding of how metallocene catalysts operate. He showed that these principles extend broadly to other classes of catalysts. This work was a significant achievement in the development of modern single-site olefin polymerization catalysis.

Jordan has developed stereoselective syntheses of chiral metallocenes that are widely used. He discovered that cationic zirconocenes activate the C-H bonds of heterocycles and developed catalytic heterocycle/olefin coupling reactions based on this chemistry. He has also explored the chemistry of low-coordinate cationic main-group alkyls that are designed to exhibit maximum Lewis acidity, and neutral olefin polymerization catalysts based on carborane ligands. Jordan's current efforts are focused on the "polar monomer problem," i.e. the challenge of developing insertion polymerization catalysts that can incorporate functionalized monomers in olefin polymerization, enabling the direct synthesis of functionalized polyolefin plastics.

Jordan has authored approximately 190 publications and 14 patents and has given 350 invited lectures at conferences, universities and companies. He has served on the Editorial Advisory Boards of *Organometallics* and the *Journal of Organometallic Chemistry*, the Board of Directors of the University of Iowa Research Foundation and the Governing Board of the Council for Chemical Research. He is a Fellow of the AAAS and was the Chair of the Organometallic Subdivision of the ACS (1998) and Chairman of the 2010 Gordon Research Conference on Organometallic Chemistry. He was an Alfred P. Sloan Research Fellow, a Union Carbide Research Innovation Awardee, and a visiting professor at the University of Rennes and Zhejiang University. Jordan has served as a consultant for and participated in research collaborations with numerous industrial organizations.



## RICHARD R. SCHROCK

Massachusetts Institute of Technology  
Monday, October 22, 2012; 1:10 PM

Richard R. Schrock was born in Indiana, but spent his high school years in San Diego, California, and obtained his B.A. degree in 1967 from the University of California at Riverside. He attended graduate school at Harvard University, from which he received his Ph.D. degree in inorganic chemistry in 1971 (awarded 1972) as a student of J. A. Osborn. He spent one year as an NSF postdoctoral fellow at Cambridge University working in the group of Lord Jack Lewis. In 1972 he accepted a position in the group of George Parshall at the Central Research and

Development Department of E. I. duPont de Nemours and Company. He moved to M.I.T. in 1975 where he became full professor in 1980 and in 1989 the Frederick G. Keyes Professor of Chemistry. Schrock has been an Alfred P. Sloan Fellow, a Camille and Henry Dreyfus Teacher-Scholar, the Royal Society Centenary Lecturer and Medalist in 1991, an Alexander von Humboldt Fellow (1995), the Sir Geoffrey Wilkinson Lecturer and Medalist (2002), and the Sir Edward Frankland Prize Lecturer (2004). He has received the ACS Award in Organometallic Chemistry (1985), the Harrison Howe Award of the Rochester ACS section (1990), the ACS Award in Inorganic Chemistry (1996), the Bailar Medal from the University of Illinois (1998), an ACS Cope Scholar Award (2001), the ACS Cotton Award (2006), the August Wilhelm von Hofmann Medal from the German Chemical Society (2005), and the Theodore W. Richards Medal (2006). In 2005 he received the Nobel Prize in chemistry in 2005 with R. H. Grubbs and Y. Chauvin. He has been elected to the American Academy of Arts and Sciences and the National Academy of Sciences, and is a Foreign Member of the Royal Society of London. He has published more than 525 research papers, and supervised over 150 Ph.D. students and postdocs. Schrock is best known as the discoverer of  $\alpha$  hydrogen abstraction reactions in high oxidation state metal alkyl complexes that yield "high oxidation state" alkylidene and alkylidyne complexes, and for synthesizing those that are active for olefin and alkyne metathesis, respectively. His current interests include syntheses of new molybdenum and tungsten alkylidene complexes and application of olefin metathesis reactions in organic and polymer (ROMP) chemistry. His other notable achievement is the catalytic reduction of dinitrogen at a well-defined molybdenum catalyst center with protons and electrons.

### **Abstract: Molybdenum and Tungsten Catalysts for Selective Olefin Metathesis Reactions**

In the last five years we have discovered and developed "third generation"  $M(NR)(CHCMe_2R')(OR)(Pyr)$  (MonoAlkoxidePyrrolide or MAP;  $M = Mo$  or  $W$ ) catalysts for olefin metathesis. MAP complexes are excellent catalysts for *Z*- and enantioselective ring-opening/cross-metatheses, ethenolysis of internal olefins in natural feedstocks such as oleic acid esters, *Z*-selective coupling of terminal olefins, *Z*-selective cross coupling of terminal olefins, and formation of macrocycles *Z*-selectively. Ethenolysis has also been shown to be *Z*-selective, a fact that allows pure *E* olefins to be prepared through selective destruction of the *Z* olefin in thermodynamic *E/Z* mixtures. Therefore, *E* olefins can be prepared from terminal olefins in a two step process. *Z*-selective catalysts also initiate ROMP (Ring Opening Metathesis Polymerization) to give polymers that have a single structure. I will focus on the synthetic and mechanistic organometallic chemistry of MAP species and on new synthetic approaches to metathesis catalysts as time permits.





## PAUL J. CHIRIK

Princeton University

Monday, October 22, 2012; 2:00 PM

Paul Chirik earned his B.S. in Chemistry from Virginia Tech in 1995 and Ph.D. from Caltech in 2000 as a student of John Bercaw. For his thesis work, he was awarded the Hebert Newby McCoy award. After a postdoctoral appointment with Professor Christopher Cummins at MIT, Chirik began his independent career at Cornell University in 2001. In 2006, he was promoted to Associate Professor and in 2009 was named the Peter J. W. Debye Professor of Chemistry. In 2011, Chirik and his research group moved to

Princeton University where he was named the Edward S. Sanford Professor of Chemistry. He has been recognized with an Arthur C. Cope Scholar Award by the American Chemical Society, the Blavatnik Award for Young Scientists by the New York Academy of Sciences, a Packard Fellowship in science and engineering, a Camille Dreyfus Teacher Scholar Award, a Bessel Fellow of the Alexander von Humboldt Foundation and an NSF CAREER Award. In 2010-2011, Chirik has also served as a member of the Defense Science Study Group – a collection of early career academics exploring science and technology issues related to national security. He is currently an Associate Editor of *Catalysis Science and Technology*.

### **Abstract: Modern Alchemy: The Chemistry of Base Metal Catalysis**

Transition metal catalyzed reactions have revolutionized the art of chemical synthesis. Applications range from the selective synthesis of single enantiomer drugs to the bulk production of high performance silicones. In most cases, these reactions rely on second and third row metals such as Pt, Pd, Rh, and Ir, which are expensive and toxic. My lecture will focus on replacing these metals more environmentally benign and inexpensive iron and cobalt compounds. Our strategy has focused on so-called "redox-active ligands" – those that undergo reversible electron transfer with the metal. This concept is used to suppress the radical chemistry of the base metals and "transmute" the electronic structure of the first row ions into those more familiar with the heavy metals. Applications such as alkene hydrosilylation, asymmetric olefin hydrogenation and more unique cycloaddition chemistry will be presented. One illustrative example is the hydrosilylation of  $\alpha$ -olefins. With iron catalysts, highly selective anti-Markovnikov additions are observed and have application in the industrial production of agrochemical compounds, tires and personal care ingredients. As will be highlighted, we have discovered that the base metals, likely by virtue of their unusual electronic structures, offer unique chemistry that has not been observed with their heavier congeners.



## CHRISTOPHE COPÉRET

ETH Zürich

Monday, October 22, 2012; 3:05 PM

Prof. Christophe Copéret (CCH) was trained in chemistry and chemical engineering in CPE Lyon (France) and then undertook a PhD in chemistry at Purdue University (USA), where he studied the development of highly efficient synthesis of complex molecules via Pd-catalyzed carbonylation reactions in the group of Prof. E.i. Negishi (1991-1996). After a postdoctoral stay at the Scripps Research Institute (La Jolla, USA) in the group of Prof. K.B. Sharpless (1996-1997), where he developed oxidation reactions, CCH was offered in

1998 a permanent research position in CNRS in C2P2, a laboratory devoted to catalysis, chemistry of surfaces and polymers, and was promoted CNRS Research Director in 2008. Since November 1, 2010, CCH has been a Professor in the Department of Chemistry (Institute of Inorganic chemistry) at ETH Zürich. CCH obtained the CNRS Young investigator award in 2001 and was the Seaborg lecturer 2012 at UC Berkeley. His scientific interest lies at the frontiers of molecular, material and surface chemistry, with the aims to design functional materials with applications in catalysis (sustainable chemistry and energy), molecular recognition, imaging and microelectronics. Besides scientific activities, CCH enjoys literature, history, cooking and wine tasting, probably a reminiscence of his childhood spent in the vineyards in [Fleurie](#), one of the famous crû of Beaujolais (La reine) just 50 km North of Lyon.

### **Abstract: Controlled Functionalization of Surfaces: Supported Single-Site Catalysts and Beyond**

Homogeneous and heterogeneous catalysts have, each, specific advantages. While homogeneous catalysts are typically associated with efficient chemical transformations at low temperatures (high selectivity), heterogeneous ones are typically preferred in term of processes (easier regeneration and separation processes).

Here, we will show how it is possible to combine the advantages of homogeneous and heterogeneous catalysts by the controlled functionalization of the surfaces of oxide materials and by the characterization of surface species at the molecular level, thus allowing more predictive approaches.

We will illustrate the power of this approach with the development of well-defined "single-sites", whose performance and stability can be far above those displayed by homogeneous and heterogeneous catalysts, *e.g.* alkene metathesis.<sup>2</sup>

With our current level of understanding of surfaces, we will also discuss new directions in this field: understanding defect sites of surfaces and metal-support interactions at the molecular level, introducing diversity in oxide chemistry, controlling the growth of nanoparticles, the development of luminescent devices, etc.



## MICHAEL J. KRISCHE

The University of Texas at Austin  
Tuesday, October 23, 2012; 8:00 AM

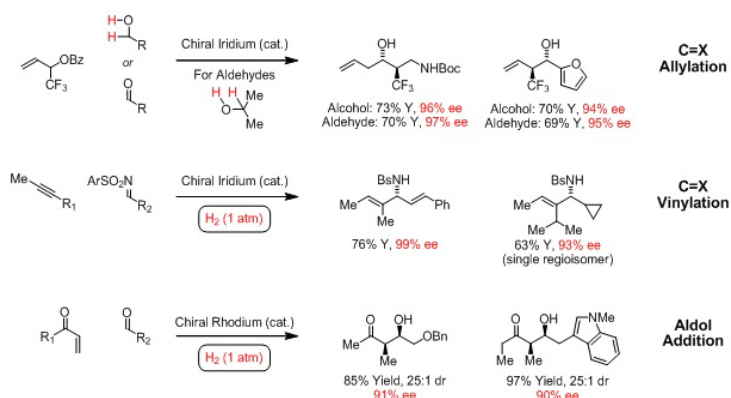
Professor Michael J. Krische obtained a B.S. degree in Chemistry from the University of California at Berkeley, where he performed research with Professor Henry Rapoport. After one year of study abroad as a Fulbright Fellow, he initiated graduate research at Stanford University with Professor Barry Trost as a Veatch Graduate Fellow. Following receipt of his Ph.D. degree, he worked with Jean-Marie Lehn at the Université Louis Pasteur as an NIH Post-Doctoral Fellow. In Fall 1999, Professor Krische was appointed Assistant

Professor at the University of Texas at Austin. He was promoted directly to Full Professor in Fall 2004. In Fall 2007, he was appointed the Robert A. Welch Chair in Science.

Selected Honors and Awards: Glaxo-Smith-Kline Scholar Award (2011), Mukaiyama Award (2010), Tetrahedron Young Investigator Award (2009), Humboldt Foundation Senior Research Award (2009), Novartis Chemistry Lectureship (2008), Presidential Green Chemistry Award (2007), Dowpharma Prize (2007), ACS Elias J. Corey Award (2007), Solvias Ligand Prize (2006), Society of Synthetic Chemistry Japan Lectureship (2005), Johnson & Johnson Focused Giving Award (2005), Dreyfus Teacher Scholar Award (2003), Alfred P. Sloan Research Fellowship (2003), Cottrell Scholar Award (2002), Frascch Foundation Award in Chemistry (2002), Lilly Grantee Award (2002), National Science Foundation-CAREER Award (2000), Maître de Conference, Collège de France (1999), NIH Post-Doctoral Fellow (1997), Veatch Graduate Fellow (1995), Sigma Xi Grantee (1991), Fulbright Fellow (1990).

Research Abstract: Under hydrogenation conditions employing chiral rhodium and iridium catalysts, diverse  $\pi$ -unsaturated reactants engage in reductive C-C coupling to carbonyl

compounds and imines, offering a byproduct-free alternative to stoichiometric organometallic reagents in a range of classical C=X (X = O, NR) addition processes. This concept is extended further by "C-C bond forming transfer hydrogenations". Here, using ruthenium or iridium catalysts, alcohols serve dually as hydrogen donors and aldehyde precursors, enabling carbonyl addition directly from the alcohol oxidation level in the absence of stoichiometric byproducts. These processes represent the first C-C bond forming hydrogenations beyond hydroformylation.



Selected Publications: "Enantioselective C-H Crotylation of Primary Alcohols via Hydrohydroxyalkylation of Butadiene," Zbieg, J. R.; Yamaguchi, E.; McInturff, E. L.; Krische, M. J. *Science* **2012**, In Press. "Direct Catalytic C-C Coupling of Methanol in Employing a Homogeneous Iridium Complex: Hydrohydroxymethylation of Allenes," Moran, J.; Preetz, A.; Mesch, R. A.; Krische, M. J. *Nature Chem.* **2011**, *3*, 287. "Iridium Catalyzed *anti*-Diastereo- and Enantioselective Carbonyl ( $\alpha$ -Trifluoromethyl)allylation from the Alcohol or Aldehyde Oxidation Level," Gao, X.; Zhang, Y. J.; Krische, M. J. *Angew. Chem. Int. Ed.* **2011**, *50*, 4173. "Diastereo- and Enantioselective Hydrogenative Aldol Coupling of Vinyl Ketones: Design of Effective Monodentate TADDOL-Like Phosphonite Ligands," Bee, C.; Han, S. B.; Hassan, A.; Iida, H.; Krische, M. J. *J. Am. Chem. Soc.* **2008**, *130*, 2747. "Enantioselective Iridium Catalyzed Imine Vinylation: Optically Enriched Allylic Amines via Alkyne-Imine Reductive Coupling Mediated by Hydrogen," Barchuk, A.; Ngai, M.-Y.; Krische, M. J. *J. Am. Chem. Soc.* **2007**, *129*, 12644.



## AMIR H. HOVEYDA

Boston College

Tuesday, October 23, 2012; 8:10 AM

Amir H. Hoveyda is the Patricia and Joseph T. '49 Vanderslice Millennium Professor and chairperson of Chemistry at Boston College. He received his B.A. degree at Columbia in 1981, and was a graduate student at Yale with Stuart L. Schreiber. After receiving his Ph.D. in 1986, he joined David Evans at Harvard as an American Cancer Society postdoctoral fellow. In June 1990, Hoveyda joined the faculty at Boston College, where he was promoted to rank of Professor in 1994; in 1998, he was appointed to his present position.

Hoveyda's honors include an NSF National Young Investigator Award (1992), an Eli Lilly Young Investigator Award (1992), a Pfizer Award in Synthetic Organic Chemistry (1993), an Alfred P. Sloan Fellowship (1994), a Camille Dreyfus Teacher-Scholar Award (1994), ACS Cope Scholar Award (1998), the 2002 ExxonMobil Award for Excellence in Catalysis, an NIH MERIT Award (2005), the 2007 Max Tishler Prize and the 2010 Yamada-Koga Prize. Hoveyda's research interests are in the discovery and development of new catalysts and stereoselective reaction methods, organometallic chemistry, study of reaction mechanisms, enantioselective catalysis and synthesis of complex natural products. He has published more than 200 research articles and is the co-founder of XiMo, Inc. (with Richard Schrock).

### **Abstract: New Concepts, Catalysts and Methods for Stereoselective Synthesis of Alkenes. Mechanistic Insights and Applications to Complex Molecule Synthesis**

The need for reliable catalysts, methods and methods for efficient and stereoselective formation of alkenes, perhaps the most versatile functional group in organic chemistry, represents an important and difficult challenge in chemical synthesis. Particularly uncommon are protocols that are catalytic and deliver thermodynamically less favored Z alkenes. Catalytic olefin metathesis offers exceptionally efficient pathways for synthesis of C–C double bonds; cross- and ring-closing metathesis, reactions that generate the easily removable ethylene as the side-product, constitute remarkably efficient strategies for olefin synthesis. What renders the goal of a Z-selective olefin metathesis processes especially daunting is that not only must the catalyst generate the higher energy isomer preferentially, it must do so without inflicting significant post-metathesis isomerization, which would result in the erosion of the hard-earned kinetic selectivity.

In this lecture, the first examples of exceptionally efficient and highly Z-selective catalytic cross-metathesis and ring-closing metathesis reactions will be presented. It will be demonstrated that, through utilization of unique structural attributes of different types of metal-based catalysts, reactivity and selectivity levels that were previously entirely out of reach can be attained. Principal design principles leading to the development of such catalysts, mechanistic insights offered by examining the corresponding transformations as well as applications to total synthesis of several complex molecules of significance to biology and medicine will be presented.



## F. DEAN TOSTE

University of California, Berkeley  
Tuesday, October 23, 2012; 9:00 AM

F. Dean Toste was born in Terceira, Azores, Portugal but soon moved to Toronto Canada. He received his B.Sc. and M.Sc. degrees in chemistry from the University of Toronto, Canada where he worked with Prof. Ian W.J. Still. In 1995, he began his doctoral studies at Stanford University under the direction of Professor Barry M. Trost. Following postdoctoral studies with Professor Robert H. Grubbs at Caltech, he joined the faculty at the University of California, Berkeley in July of 2002, and was promoted to Associate Professor in 2006 and

Professor in 2009. Professor Toste's honors include an Alfred P. Sloan Research Fellowship (2005), the Cope Scholar Award (2006) and the E.J. Corey Award (2008) from the American Chemical Society, BASF Catalysis Award (2007) and the OMCOS (2007) and Thieme Award (2008) from IUPAC, the Merck Award (2010) from the Royal Society of Chemistry, the Mukaiyama Award (2011) and the Tetrahedron Award (2011) and numerous awards from the pharmaceutical industry.

### Abstract: Enantioselective Catalysis with Gold Complexes

This lecture will focus on the development of gold(I) complexes for enantioselective catalysis.

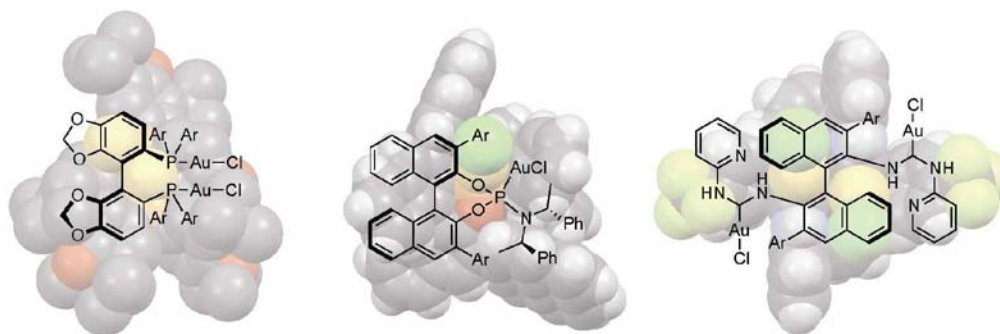


Figure 1. Catalysts for Gold(I)-Catalyzed Enantioselective Transformations

Most prominently the use of bisphosphine-,<sup>[1]</sup> phosphoramidite-,<sup>[2]</sup> and biscalbene<sup>[3]</sup>-gold(I) complexes (Figure 1) as catalysts will be discussed. The use of chiral anions,<sup>[4]</sup> with achiral gold complexes, as an alternative strategy to the use of chiral ligands will also be presented. The application of these complexes as catalysts for enantioselective cyclopropanation, heterocyclization, rearrangement, cycloaddition and protonation reactions will be discussed. Particular attention will be devoted to the mechanistic hypotheses that form the basis for catalyst discovery and the development of new reactions.

### References

- [1] M. J. Johansson, D. J. Gorin, S. T. Staben, F. D. Toste, *J. Am. Chem. Soc.* **127**, 18002 (2005).
- [2] A. Z. Gonzalez, D. Benitez, E. Thatchouk, W. A. Goddard, F. D. Toste, *J. Am. Chem. Soc.* **133**, 5500 (2011).
- [3] Y-M. Wang, C. N. Kuzniewski, V. Rauniyar, C. Hoong, F. D. Toste, *J. Am. Chem. Soc.* **133**, 12972 (2011).
- [4] G. L. Hamilton, E. J. Kang, M. Mba, F. D. Toste, *Science* **317**, 496 (2007).



## **VY M. DONG**

University of Toronto

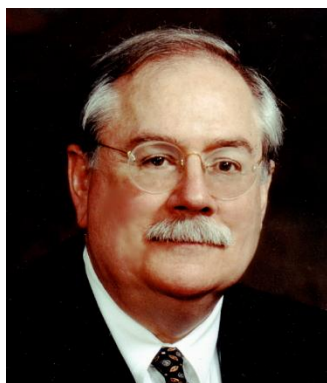
Tuesday, October 23, 2012; 10:05 AM

Vy M. Dong was born in Big Spring, Texas and spent early childhood in west Texas before moving with family to southern California. She graduated magna cum laude from the University of California at Irvine where she majored in chemistry and completed an honor's thesis with Larry Overman. After graduation, she joined David MacMillan's group at UC Berkeley, and then moved with his group to the California Institute of Technology to complete her doctoral studies. Her doctoral work featured variants of the zwitterionic-

Claisen rearrangement and a total synthesis of erythronolide B. As an NIH postdoctoral fellow, Vy returned to Berkeley to obtain training in organometallic and supramolecular chemistry with Robert Bergman and Kenneth Raymond. In 2006, she began an independent career at the University of Toronto where she was promoted with tenure and named the Adrian Brook Distinguished Professor. The Dong research group specializes in organic synthesis and transition metal-catalysis. Professor Dong is recent recipient of the Roche Excellence Award in Chemistry, Eli Lilly Grantee Award, and the American Chemical Society Arthur C. Cope Scholar Award.

### **Abstract: A Few of My Favorite Rings: Catalysis Inspired by Lactones and Lactams**

Lactones and lactams make up a range of structurally complex and functional compounds, from antibiotics to nanomaterials. Inspired by Nature's cyclic architectures, we are developing catalytic methods that feature stereoselective hydroacylation. Hydroacylation, the formal addition of an aldehyde C–H bond across an unsaturated functional group, is an ideal approach to carbonyl functionalities commonly found in bioactive molecules. We aim to advance hydroacylation as a unified strategy for transforming aldehydes into chiral esters, ketones, and amides. In this context, my lecture will discuss the design, scope, and mechanism for hydroacylation methods using both rhodium and ruthenium catalysis. Our long-term goal is to develop more green, versatile, and efficient strategies for constructing heterocycles, polyketides, and other biologically relevant motifs.



## DAVID A. EVANS

Harvard University

Tuesday, October 23, 2012; 10:55 AM

David A. Evans was born in Washington, D.C. in 1941. He received his A.B. degree from Oberlin College in 1963 where he concentrated in organic and physical chemistry and worked under the direction of Professor Norman Craig for three years in the general area of vibrational spectroscopy. He subsequently obtained his Ph.D. at the California Institute of Technology in 1967, where he worked under the direction of Professor Robert E. Ireland in the general area of organic synthesis. In that year he joined the faculty at the University of California, Los Angeles. In 1973 he was promoted to the

rank of Full Professor and shortly thereafter returned to Caltech where he remained until 1983. In that year he joined the Faculty in the Chemistry Department at Harvard University, and in 1990 he was appointed as the Abbott and James Lawrence Professor of Chemistry. In July 1998 he completed his three-year term as the Department Chair, and in the following year he was named Research Professor.

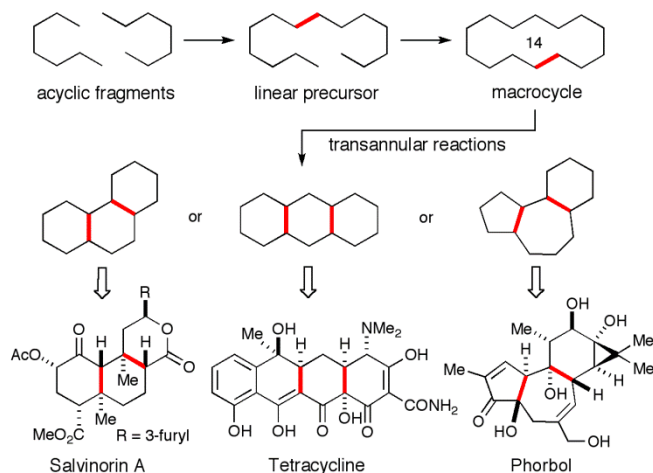
Professor Evans has been the recipient of numerous honors: ACS Award for Creative Work in Synthetic Organic Chemistry (1982); Arthur C. Cope Scholar Award (1988); Yamada Prize (1997); Tetrahedron Prize (1998); Robert Robinson Award, Oxford Univ. (1998); Tetrahedron Prize (1998); Prelog Medal, ETH (1999); Arthur C. Cope Award (2000); Caltech Distinguished Alumni Award (2002); Nagoya Medal (2003); Karl Ziegler Prize, Max Planck Institute (2003); Gibbs Medal (2005); Glenn T. Seaborg Medal, UCLA (2006); and the Herbert C. Brown Award (2007). He was elected into the National Academy of Sciences in 1984, the American Academy of Arts and Sciences in 1988, Fellow, Royal Society of Chemistry in 2008, and Humboldt Senior Scientist in 2008. He also received the Phi Beta Kappa Teaching Prize for Contributions to Undergraduate Education at Harvard in 2007.

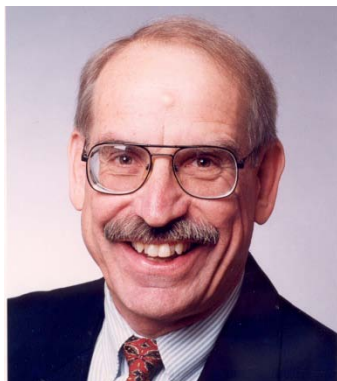
Professor Evans has made significant advances in the design of stereoselective reactions and the applications of these processes to natural products synthesis. Over the last three decades, new reaction methodology directed toward achieving absolute stereocontrol has the central theme in his laboratory. Both catalytic and auxiliary-based reactions have been developed. Enantioselective Diels-Alder, Michael, and aldol reactions are but three of the important families of processes developed in his group. In the area of synthesis design, Evans was the first to achieve the *de novo* synthesis of complex natural products through the exclusive use of chiral auxiliaries and catalysts to control absolute stereochemical relationships. This represented a dramatic departure from the more prevalent reliance on the "chiral pool" for structural components of the target structure.

### Abstract: Polycyclic Structures from Macrocyclic Intermediates

Our laboratory has spent nearly three decades developing reactions that facilitate the generation of asymmetric centers in acyclic carbon fragments. One of the obvious goals in this effort has been application to the synthesis of macrolide antibiotics. As an extension of this research program, we are now addressing the utility of assembling advanced macrocyclic intermediates that may be transformed into polycyclic ring systems through the use of selective transannular reactions.

There is an assortment of important structural motifs that may be generated from a 14-membered macrocycle. For example, we have shown that salvinorin (**1**) can be derived from a 14-membered macrocycle using two transannular Michael reactions. Alternate transannular processes could lead to the construction of the tetracycline nucleus and to tricyclic diterpenoids.





## **JOHN E. BERCAU**

California Institute of Technology  
Tuesday, October 23, 2012; 1:00 PM

John Bercau received his B.S. degree from North Carolina State University in 1967, Ph.D. from the University of Michigan in 1971, and undertook postdoctoral research at the University of Chicago. He joined the faculty at the California Institute of Technology as an Arthur Amos Noyes Research Fellow in 1972; in 1974 he joined the professorial ranks, becoming Professor of Chemistry in 1979. From 1985 to 1990 he was the Shell Distinguished Professor of Chemistry, in 1993 he was named Centennial Professor of Chemistry. Bercau has been a Seaborg Scholar at Los Alamos National Laboratory (2004); Robert Burns Woodward Visiting Professor at Harvard University (1999); George F. Baker Lecturer at Cornell University (1993); Visiting Miller Professor, University of California, Berkeley (1990), and Royal Society of Chemistry Guest Research Fellow, Oxford University (1989-1990). In 2009 he was also named KFUPM Chair Professor at King Fahd University of Petroleum and Minerals. He has served on numerous panels for the Department of Energy, the National Research Council, and beginning in 1999 a member of the University of California, Office of the President's Panels on Science and Technology for Lawrence Livermore and Los Alamos National Laboratories, and now the Science and Technology Committee for Los Alamos National Security and Lawrence Livermore National Security.

He was elected a member of the National Academy of Sciences (1990), and Fellow of the American Academy of Arts and Sciences (1991). In 2001 he was awarded an Honorary Doctorate of Science, University of Chicago. Selected a Chemical Pioneer by the American Institute of Chemists (1999). Among other honors: the American Chemical Society awards in Pure Chemistry (1980), Organometallic Chemistry (1990), Distinguished Service in the Advancement of Inorganic Chemistry (1997), George A. Olah Award for Hydrocarbon or Petroleum Chemistry (1999), and Arthur C. Cope Scholar Award (2000). He held the Sir Edward Frankland Prize Lectureship of the Royal Society of Chemistry in 1992 and received the Basolo Medal (Northwestern, 2005) and the Bailar Medal (University of Illinois, 2003).

His research interests are in synthetic, structural and mechanistic organotransition metal chemistry. Recent studies include catalysts for polymerization of olefins, investigations of hydrocarbon hydroxylation with transition metal complexes, and the development of catalysts for syngas conversion to chemicals. He has published over 260 peer-reviewed scientific articles.





## MARCETTA Y. DARENSBOURG

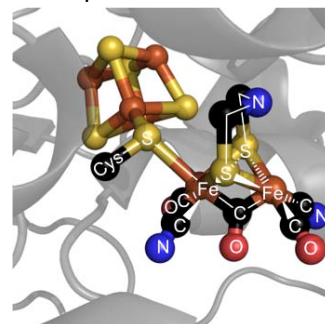
Texas A&M University

Tuesday, October 23, 2012; 1:10 PM

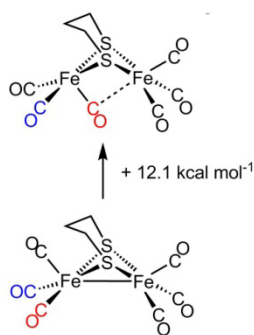
Professor Marcetta Y. Darensbourg is a native of Kentucky, USA, with a Ph.D. from the University of Illinois. Following academic posts at Vassar College and Tulane University, she joined the faculty at Texas A&M University, College Station, TX, in 1982. She holds the title of Distinguished Professor of Chemistry. Trained as an organometallic chemist and with earlier research programs in low valent transition metal hydrides, the possibility of metal hydrides in nature, specifically as intermediates in hydrogenase metalloenzymes lured her into the new field of bioorganometallic chemistry. She has been a leader in the development of synthetic analogues of the diiron hydrogenase active site and the insight they bring to the catalytic mechanism of these natural fuel cell catalysts.

### Abstract: Molecular Constructs as [FeFe]-H<sub>2</sub>ase Enzyme Active Site Biomimetics for Proton Reduction

The structurally unique diiron catalytic unit that exists in the active site of the [FeFe]-H<sub>2</sub>ase is of special interest to biomimetic/synthetic chemists as its construction exploits diatomic CO and CN<sup>-</sup> ligands, perhaps deriving from primordial iron/sulfur chemistry, rather than typical donors covalently bound to a peptide chain. Thus the torsion angles responsible for the mismatch of donor ligand-metal geometric preferences that lead to high rates of catalysis in classical transition metal biocatalysts are minimal in such organometallics. These features, along with the ease of modifying a simple precursor, (μ-S(CH<sub>2</sub>)<sub>3</sub>S)[Fe(CO)<sub>3</sub>]<sub>2</sub>, that has core features of the [FeFe]-H<sub>2</sub>ase enzyme active site (eas), and the possibility to develop base metal catalysts for fuel cell use, have attracted a new coterie of chemists to biomimetic synthesis. They bring the spectroscopic tools and structure/bonding approaches of organometallic chemistry to bear on defining the features that are the primary differences



between the eas and the parent model. Despite the simplicity of (μ-S(CH<sub>2</sub>)<sub>3</sub>S)[Fe(CO)<sub>3</sub>]<sub>2</sub>, modifications abound that lead to closer analogues of the eas diiron unit. They include positioning a bridgehead amine for proton shuttling in the S to S linker as is found in the eas, and exchange of CO for cyanide. Some of the models are electrocatalysts for proton reduction, but not with the efficiency of the enzyme.



In contrast to the symmetrical thiolate sulfur edge-bridged square pyramidal structure of the parent model which accommodates an Fe<sup>I</sup>-Fe<sup>I</sup> bond, the eas has one square pyramid inverted with respect to the other, disrupting the Fe-Fe bond and creating an open site on a terminal iron where hydrogen chemistry may occur. This lecture will describe approaches to stabilize and isolate the unusual « rotated » structure, and insight gained into Nature's choice of the diiron construct.



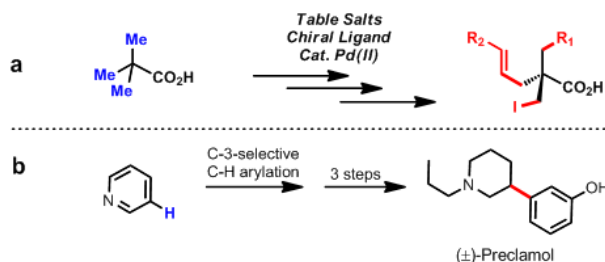
## JIN-QUAN YU

The Scripps Research Institute  
Tuesday, October 23, 2012; 2:15 PM

Jin-Quan Yu earned his B.S. in Chemistry in 1987, at East China Normal University, Shanghai, his M.S. in Organic Chemistry in 1990, at the Guangzhou Institute of Chemistry, Guangzhou, China and his Ph.D. in Organic Chemistry in 1999, at Cambridge University, Cambridge, UK, under the direction of Professor J. B. Spencer. Dr. Yu completed his postdoctoral fellowship at Harvard University in 2002, under the direction of Professor E. J. Corey. From 2003 – 2004 Dr. Yu was a Royal Society Research Fellow at the University of Cambridge, UK, and from 2004 – 2006 he held the position of Assistant Professor in the Department of Chemistry at Brandeis University in Waltham, Massachusetts. In 2007 he began his position as a Tenured Associate Professor in the Department of Chemistry at The Scripps Research Institute, and in August of 2010 he was promoted to Full Professor in the Department of Chemistry, The Scripps Research Institute. Dr. Yu is the author of over 100 peer reviewed manuscripts, and is the recipient of the Mukaiyama Award from the Society of Organic Synthesis, (Japan, 2012); the ACS Cope Scholar Award (2012); the Novartis Early Career Award in Organic Chemistry (2011); the Hirata Memorial Lectureship Award (2011); and the Amgen Young Investigator's Award (2008), to name a few.

### Abstract: Accelerated C-H Activation Reactions: A Shortcut to Drug Molecules from Chemical Feedstock

Pd(II)-catalyzed enantioselective and position-selective C–H activation reactions are developed using mono-*N*-protected chiral amino acid ligands. C–H activation intermediates are characterized, offering insights into the origin of the observed stereoselectivity. Most importantly, these chiral ligands are found to accelerate drastically C–H activation reactions, shortening the reaction time from two days to 20 minutes.





## MAURICE BROOKHART

University of North Carolina at Chapel Hill

Tuesday, October 23, 2012; 3:05 PM

Maurice Brookhart (b. 1942) grew up in the mountains of western Maryland and attended Johns Hopkins University in Baltimore where he received an A.B. degree in chemistry in 1964. He carried out his doctoral work in physical organic chemistry at UCLA under the direction of Saul Winstein. After finishing the Ph.D. degree in 1968, he spent six months as a National Science Foundation postdoctoral fellow at UCLA with Winstein and Frank Anet, followed by a year of study at Southampton University as a NATO postdoctoral fellow.

Brookhart joined the University of North Carolina faculty in 1969 and is currently a William R. Kenan, Jr. professor of chemistry. He has spent research leaves at Univ. of Rennes (1981), Oxford (1982-83), UC-Berkeley, (Fall, 1996), Seville (Spring, 1997), University of Marburg (Spring, 2001) and the Max Planck Institute, Muelheim (Spring, 2003). Brookhart served as associate editor of *Organometallics* (1990-96) and received the 1992 American Chemical Society (ACS) Award in Organometallic Chemistry, a 1994 ACS Cope Scholar Award and the 2003 ACS Award in Polymer Chemistry. He was elected to the American Academy of Arts and Sciences in 1996 and the National Academy of Sciences in 2001 and received the North Carolina Award in Science in 2008 and the Willard Gibbs Medal in 2010.

Brookhart's research interests span mechanistic, synthetic, and structural organometallic chemistry. Most recently efforts have focused on the development and mechanistic understanding of late transition metal complexes for olefin polymerizations and employing C-H and Si-H bond activation processes in catalytic transformations of small molecules, particularly hydrocarbons.

### **Abstract: Applications of Iridium Pincer Complexes in Catalysis: Hydrocarbon Conversions**

There are now numerous transition metal-based systems known that will activate carbon-hydrogen bonds of alkanes via oxidative addition reactions. Only a few such reactions have been incorporated into viable, efficient catalytic cycles. This presentation will focus on the use of iridium pincer complexes for catalytic transformations in which C-H bond activation is the key step. These processes will include: 1. intermolecular transfer dehydrogenation reactions as a method for introducing carbon-carbon double bonds into alkanes and 2. coupling such reactions with alkene metathesis to provide a method for converting alkanes to linear alkanes of higher and lower carbon number (alkane metathesis). Transfer dehydrogenation chemistry employing ethylene as an acceptor has been coupled with a Diels-Alder reaction to provide a method of synthesizing *para*-xylene, a high volume aromatic intermediate, from ethylene as the sole feedstock. The alkane metathesis process can potentially be used for converting light alkanes generated via the Fischer-Tropsch process to alkanes in the diesel range, thus providing increased efficiency for producing transportation fuels from coal, natural gas or biomass. Homogeneous and supported catalysts will be described and mechanistic aspects of these processes will be highlighted.